

# Ground-state correlation properties of charged bosons trapped in strongly anisotropic harmonic potentials

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**Abstract.** We study systems of a few charged bosons contained within a strongly anisotropic harmonic trap. A detailed examination of the ground-state correlation properties of two-, three-, and four-particle systems is carried out within the framework of the single-mode approximation of the transverse components. The linear correlation entropy of the quasi-1D systems is discussed in dependence on the confinement anisotropy and compared with a strictly 1D limit. Only at weak interaction the correlation properties depend strongly on the anisotropy parameter.

## 1 Introduction

Systems of few interacting particles confined by an external potential are of increasing interest in view of their application to model various nanostructures fabricated in an artificial way. The Schrödinger equation for harmonically trapped particles which interact through a Coulomb potential can be used to simulate different physical systems, such as semiconductor quantum dots [1] or electromagnetically trapped ions [2]. Besides of fermionic systems, also the bosonic ones have been thus considered in various theoretical contexts both in the 3D [3,4,5] and 2D [6] case. The properties of quasi-1D systems are, however, rather rarely studied, except for the models of bosons with a contact potential [7,8,9,10,11,12,13]. In this work, we discuss the case of  $N$  identically charged spinless bosons confined in a quasi-1D trap. Such a trapping potential may be experimentally realized using highly anisotropic harmonic traps where the radial confinement is much tighter than the axial one.

We discuss the effects of both the number of particles and the control parameters of the system on the correlation properties. We consider various characteristics such as single-particle reduced density matrix, single-particle density, and linear entropy. In particular, the influence of the anisotropy on the correlations within a quasi-1D structure is investigated.

Our paper is organized as follows. In Section 2 we present the model and provide an analytical formula for the effective interaction potential. Section 3 surveys the quantities we use to characterize correlations in the system. In section 4 the limit of  $\epsilon \rightarrow \infty$  is discussed. The results are presented in Section 5 and a summary of our conclusions is given in Section 6.

## 2 Effective Hamiltonian

Consider a system of  $N$  Coulombically interacting particles trapped in a 3D axially-symmetric harmonic potential with a Hamiltonian given by

$$H = \sum_{i=1}^N \left[ -\frac{\hbar^2 \nabla_i^2}{2m} + \frac{m}{2} (\omega_x^2 x_i^2 + \omega_\perp^2 \rho_i^2) \right] + \sum_{i<j} \frac{\gamma}{|\mathbf{r}_i - \mathbf{r}_j|}, \quad (1)$$

where  $\rho_i = \sqrt{y_i^2 + z_i^2}$ . After the scaling  $\mathbf{r} \mapsto \sqrt{\frac{\hbar}{m\omega_x}} \mathbf{r}$ ,  $E \mapsto \hbar\omega_x E$ , the Schrödinger equation takes the form

$$H\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = E\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N), \quad (2)$$

with

$$H = \sum_{i=1}^N \left[ -\frac{\nabla_i^2}{2} + \frac{1}{2} x_i^2 + \frac{1}{2} \epsilon^2 \rho_i^2 \right] + \sum_{i<j} \frac{g}{|\mathbf{r}_i - \mathbf{r}_j|}. \quad (3)$$

The dimensionless coupling  $g = \gamma \sqrt{\frac{m}{\omega_x \hbar^3}}$  represents the ratio of the Coulomb interaction to the longitudinal trapping energy scale and the dimensionless parameter  $\epsilon = \frac{\omega_\perp}{\omega_x}$  measures the anisotropy of the trap. We focus our attention on the strong anisotropy case,  $\epsilon \gg 1$ , when the system becomes quasi-1D. In this case the particles may be assumed to stay in the lowest energy state of the transverse Hamiltonian  $H_\perp = -\frac{\nabla_\perp^2}{2} + \frac{1}{2} \epsilon^2 \rho^2$  and the one-mode approximation is justified. The  $N$ -body wave function may be taken in the form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) \cong \psi(x_1, x_2, \dots, x_N) \prod_{i=1}^N \varphi(y_i) \varphi(z_i), \quad (4)$$

where  $\varphi(z) = \left(\frac{\epsilon}{\pi}\right)^{\frac{1}{4}} e^{-\frac{\epsilon^2}{2} z^2}$  and  $\psi$  is assumed to be a real function. After substituting (4) into (2), multiplying it

from the left by  $\varphi(y_1)\varphi(z_1)\dots\varphi(y_N)\varphi(z_N)$  and integrating over  $y_1, y_2, \dots, y_N, z_1, z_2, \dots, z_N$  we arrive at

$$H_{1D}\psi(x_1, x_2, \dots, x_N) = E_{1D}\psi(x_1, x_2, \dots, x_N), \quad (5)$$

where the quasi-1D Hamiltonian has a form

$$H_{1D} = \sum_{i=1}^N \left[ -\frac{1}{2} \frac{\partial^2}{\partial x_i^2} + \frac{1}{2} x_i^2 \right] + \sum_{i<j} g U_{1D}(x_i, x_j) + N\epsilon. \quad (6)$$

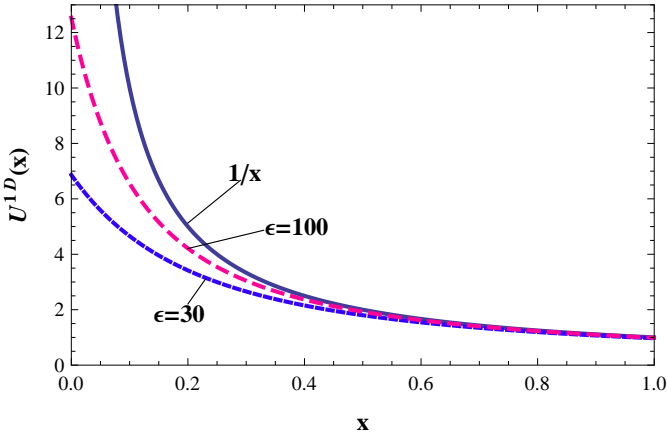
The effective interaction potential

$$U_{1D}(x_1, x_2) = \int \frac{[\varphi(y_1)\varphi(y_2)\varphi(z_1)\varphi(z_2)]^2}{|\mathbf{r}_1 - \mathbf{r}_2|} dy_1 dy_2 dz_1 dz_2 \quad (7)$$

is calculated to be given by

$$U_{1D}(x_1, x_2) = \sqrt{\frac{\epsilon\pi}{2}} e^{\frac{\epsilon(x_2-x_1)^2}{2}} (1 - \text{erf}[\sqrt{\frac{\epsilon}{2}}|x_2-x_1|]), \quad (8)$$

where  $\text{erf}(z)$  is the error function. In Fig. 1 the effective potential (8) is compared with the pure Coulomb potential for different values of  $\epsilon$ . We can notice that the larger is the value of  $\epsilon$ , the closer to the origin does the effective potential begin to exhibit Coulomb behaviour.

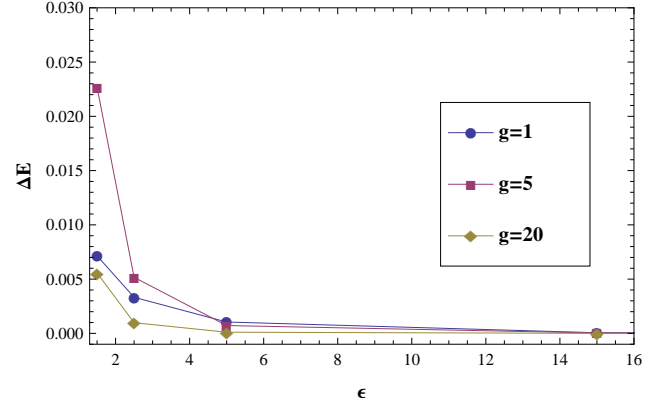


**Fig. 1.** Effective interaction potential (8) as a function of  $x = x_2 - x_1$  for the anisotropy parameter  $\epsilon = 30, 100$  compared with the Coulomb potential  $x^{-1}$ .

We have tested the applicability of the single mode approximation for the two-particle system ( $N = 2$ ) by comparing the ground-state energy  $E_{1D}$  obtained from the 1D Hamiltonian (6) with the energy  $E$  determined from the full 3D Hamiltonian (3). The relative error  $\Delta E = (|E - E_{1D}|)/E_0$  as a function of  $\epsilon$  is shown in Fig. 2 for different values of the coupling constant. One can conclude that anisotropy ratios  $\epsilon \gtrsim 5$  are sufficiently large for employing the single mode approximation.

### 3 Correlation characteristics

A basic tool to investigate two-body correlations in the system is the one-particle reduced density matrix (RDM)[14]



**Fig. 2.** Relative ground-state energy error  $\Delta E = |E - E_{1D}|/E$  as a function of  $\epsilon$  for  $N = 2$  and  $g = 1, 5, 20$ .

for spinless particles defined as

$$\rho(\mathbf{r}, \mathbf{r}') = \int \dots \int \Psi(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N) \Psi(\mathbf{r}', \mathbf{r}_2, \dots, \mathbf{r}_N) d^3\mathbf{r}_2 \dots d^3\mathbf{r}_N. \quad (9)$$

In the one-mode approximation (4) the RDM takes the form

$$\rho(\mathbf{r}, \mathbf{r}') = \varphi(y)\varphi(y')\varphi(z)\varphi(z')\rho_{1D}(x, x'), \quad (10)$$

with the 1D effective RDM given by

$$\rho_{1D}(x, x') = \int \dots \int \psi(x, x_2, \dots, x_N) \psi(x', x_2, \dots, x_N) dx_2 \dots dx_N. \quad (11)$$

The effective RDM can be represented in the Schmidt form

$$\rho_{1D}(x, x') = \sum_{l=0}^{\infty} \lambda_l v_l(x) v_l(x'), \quad (12)$$

where  $\{v_l(x)\}$  are the natural orbitals and their occupancies  $\{\lambda_l\}$ . We will concentrate on discussing the linear entropy

$$L = 1 - \int \int \rho_{1D}(x, x')^2 dx' dx. \quad (13)$$

which can be expressed in terms of  $\lambda_l$  as  $L = 1 - \sum_l \lambda_l^2$ . It gives indication of the spread of terms in the Schmidt decomposition (12) and is one of the popular measures of correlation [15,16,17,18].

### 4 Strictly 1D limit

In the strictly 1D limit of  $\epsilon \rightarrow \infty$ , the interaction potential of the considered system,  $g/|x_i - x_j|$ , diverges at  $x_i = x_j$  for any finite  $g$ . This causes divergences at short distances in calculating the energy of bosonic systems. Usually those divergences are cured by performing calculation for an anisotropic 3D system with finite  $\epsilon$  and observing the limiting behavior at  $\epsilon \rightarrow \infty$ . However, as noticed recently [19],

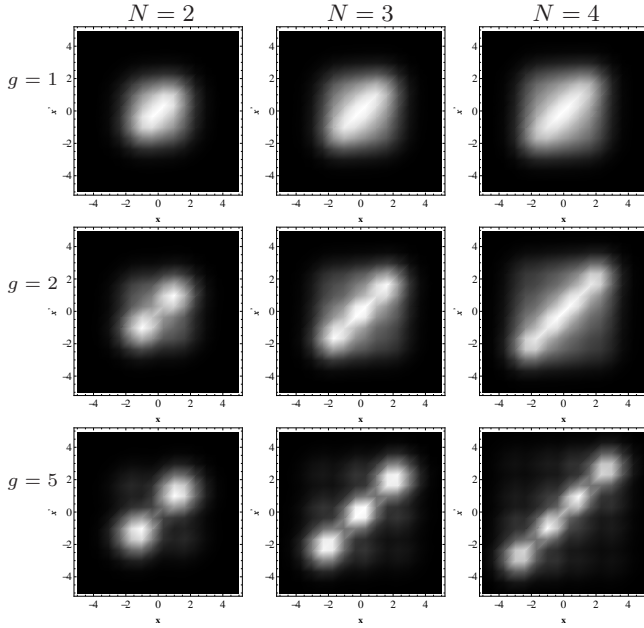
the calculation may be performed directly for the 1D system since its ground-state wavefunction can be related via Bose-Fermi mapping to the lowest energy antisymmetric  $N$ -particle wavefunction  $\psi_F$  as

$$\psi(x_1, x_2, \dots, x_N) = |\psi_F(x_1, x_2, \dots, x_N)|. \quad (14)$$

Therefore, the system of bosons gets fermionized and the ultraviolet divergencies are cured in a natural way when determining  $\psi_F$  by the standard configuration interaction method.

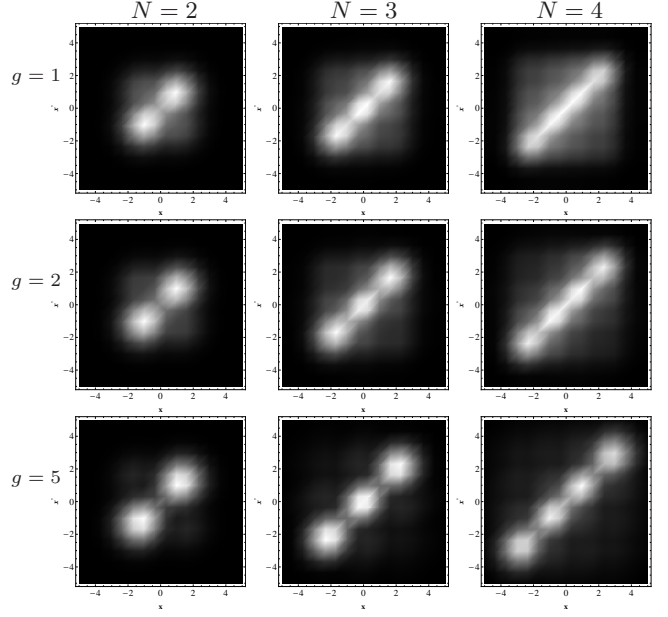
## 5 Results and discussions

We shall consider the ground-state of many-body systems with the number of particles  $N = 2, 3$  and 4. In order to reveal qualitatively the nature of correlations in the quasi-1D limit, we first discuss the case of large anisotropy,  $\epsilon = 30$ . The ground-state  $N$ -particle wave function of the Hamiltonian (6) is calculated with the quantum diffusion algorithm [20] and used to determine  $\rho(x, x')$  by numerical integration of Eq. (11).



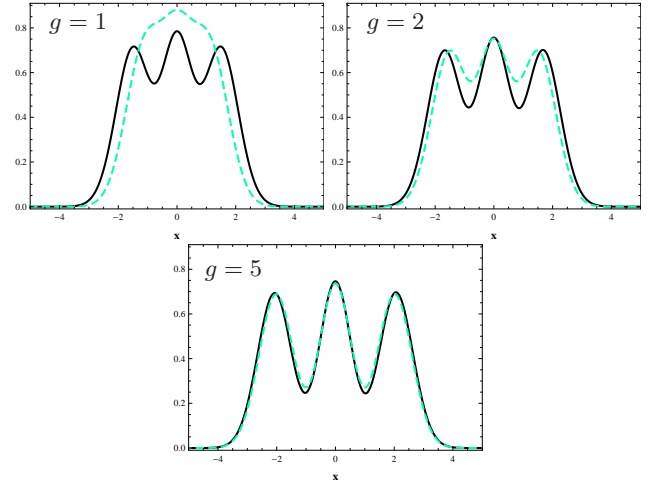
**Fig. 3.** Gray-scale plots of the effective RDM for systems of  $N = 2, 3$  and 4 particles with confinement anisotropy  $\epsilon = 30$  at various interaction strengths  $g$ .

Grey-scale plots of  $\rho(x, x')$  for the considered systems are shown in Fig. 3 at three values of the interaction strength  $g$ . As one can see, the off-diagonal elements of the RDM diminish with increasing  $g$ , which indicates a loss of spatial coherence in the system. This is due to the repulsive nature of the interaction encouraging localization of the particles, which tend to separate from each other. A clear deviation from the circular structure  $\rho(x, x') =$



**Fig. 4.** Gray-scale plots of the effective RDM for systems of  $N = 2, 3$  and 4 particles with confinement anisotropy  $\epsilon = \infty$  at various interaction strengths  $g$ .

$\pi^{-\frac{1}{2}} e^{-\frac{(x^2 + x'^2)}{2}}$  of the noninteracting case ( $g = 0$ ) is clearly observed already at  $g = 1$ . Interestingly enough, the results of Fig. 3 show that the onset of crystallization shows up at  $g = 5$ , independently on the number of particles.



**Fig. 5.** Single-particle density of  $N = 3$  particles confined with anisotropy  $\epsilon = 30$  (dashed curve) and  $\epsilon = \infty$  for various interaction strengths  $g$ .

The results at finite anisotropy  $\epsilon = 30$  may be compared with those obtained in the strictly 1D limit that are given in Fig. 4. In this case we determined  $\psi_F$ , and thereby  $\psi_B$ , using the standard configuration interaction method based on harmonically trapped single-particle eigenfunc-

tions  $\varphi_n^{ho}$ . Comparing the results of Fig. 3 with the ones of Fig. 4, one can notice that the anisotropy parameter influences the behaviour of the RDM only in the regime of small values of  $g$ . As a matter of fact, already at  $g = 5$  the RDM calculated at  $\epsilon = 30$  reproduces quite well the one calculated in the strictly 1D limit, regardless of the number of particles. We observe that below this value an increase in the anisotropy parameter has the effect of an increase in the interparticles distances. Otherwise stated, the onset of the Wigner crystallization in the strictly 1D limit appears at value smaller than that in the case of  $\epsilon = 30$ . To make the above more clear, we present in Fig. 5 the single particle densities of the 3-particle system, corresponding to the  $N = 3$  results of Figs. 3 and 4.

Next, we explore the effect of the anisotropy parameter  $\epsilon$  on the correlation properties of systems containing  $N = 2, 3$  and 4 bosonic particles. In Fig. 6 the ground-state linear entropy  $L$  at different values of  $\epsilon$  is compared with the result obtained in the fermionized strictly 1D limit of  $\epsilon \rightarrow \infty$ . The results are presented as a function of the dimensionless parameter  $g$ .

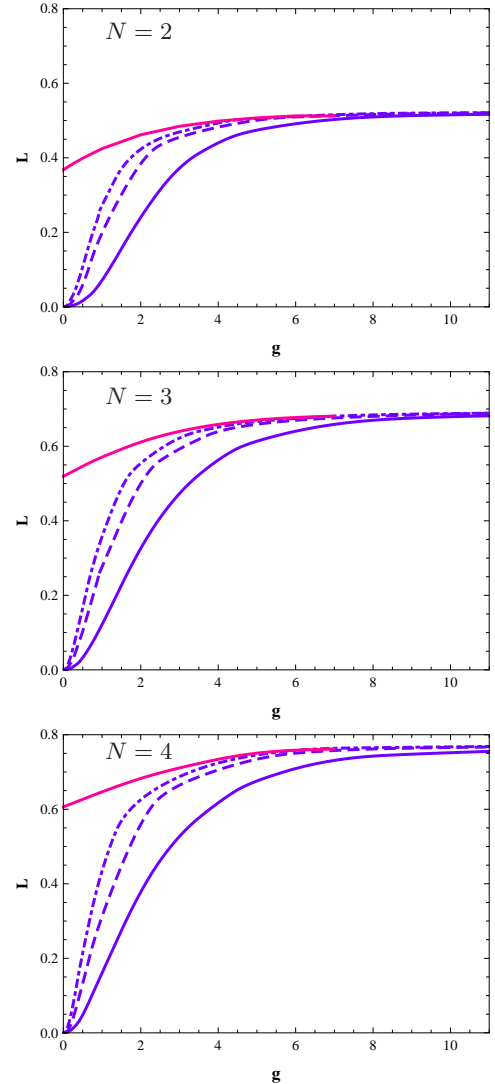
We see that in each considered case, the linear entropy increases with  $g$  and above  $g \approx 5$  saturates at a constant value that is insensitive to the anisotropy parameter  $\epsilon$ . This may be attributed to the fact that at large  $g$  the average distances between the particles are large enough so that the effective interaction exhibits pure Coulomb behaviour. The values of  $g$  at which saturation takes place seem to increase slightly with  $N$ . A look at Fig. 3 allows us to conclude that they coincide roughly with the critical values of crystallization. As can be inferred from Fig. 6, the linear entropy  $L$  increases with the number of particles in the system, with the increase getting smaller for larger  $N$ . The effect becomes less pronounced at weaker interactions and disappears in the limit of  $g \rightarrow 0$ , when  $L \rightarrow 0$ , regardless of the number of particles. At small values of  $g$ , the entropy  $L$  depends strongly on the anisotropy, being larger at larger  $\epsilon$ . Again, this can be qualitatively understood by referring to the distances of the particles, namely they are small at small values of  $g$  and are thus in the regime where the effective interaction potential (8) strongly depends on  $\epsilon$ .

The entropy in the strictly 1D limit of  $\epsilon \rightarrow \infty$  has been calculated by taking into account the Bose-Fermi mapping (14). In the limit of  $g \rightarrow 0$ , the wavefunction  $\psi_F$  reduces to a single Slater determinant and (14) takes the form

$$\psi(x_1, x_2, \dots, x_N) = \frac{1}{\sqrt{N!}} |\det_{n=0, j=1}^{N-1, N}(\varphi_n^{ho}(x_j))|. \quad (15)$$

The values of  $L_{1D}$  are calculated to be about 0.36, 0.51 and 0.6 for  $N = 2, 3$  and 4, respectively. The occurrence of fermionization for  $g \neq 0$  results in the discontinuity of the linear entropy in the point  $g = 0$ . Importantly, we observe that the smaller is  $g$  and/or  $N$  the larger is the anisotropy parameter at which the linear entropy of the quasi-1D system reaches the fermionic behaviour of the strictly 1D gas ( $\epsilon \rightarrow \infty$ ).

The asymptotic value of  $L_{1D}$  at  $g \rightarrow \infty$  can be calculated analytically in the case of  $N = 2$ , using the harmonic



**Fig. 6.** Linear entropy in the ground-state of the system of (6) for  $N = 2, 3$  and 4 particles as a function of  $g$ . Full curve,  $\epsilon = 5$ ; dashed curve,  $\epsilon = 30$ ; dot-dashed curve,  $\epsilon = 100$ . The red line is the linear entropy in the strictly 1D limit.

approximation which becomes exact in this limit [18]. The calculation analogous to that performed by us in the 2D case [18] gives

$$L_{1D}^{g \rightarrow \infty} = 1 - \sqrt{-\frac{3}{2} + \sqrt{3}} \approx 0.518, \quad (16)$$

which is in agreement with our numerical result. For  $N = 3$  and  $N = 4$  the values of  $L_{1D}^{g \rightarrow \infty}$  are found numerically to be about 0.68 and 0.77, respectively. To fully reveal the correlation effects in the strong interaction limit, it would be desirable to obtain the full dependence of  $L^{g \rightarrow \infty}$  on  $N$ . This is a topic for future investigation.

## 6 Summary

We investigated the ground-state correlation properties of the systems composed of two, three, and four particles in a strongly anisotropic harmonic trap. Within the one-mode approximation, we studied the influence of both the number of particles  $N$  and the anisotropy parameter  $\epsilon$  on the correlation properties of the systems in the whole range of repulsive interaction strength  $g$ . As a general trend we found that the linear entropy  $L$  increases with increasing  $g$ . At small  $g$  (weak interaction and/or strong confinement), the entropy of the considered systems depends heavily on the anisotropy of the trap, being larger at higher anisotropy. Linear entropy is the largest in the limit of  $\epsilon \rightarrow \infty$ , when fermionization takes place for any  $g \neq 0$ . At large  $g$  (strong interaction and/or weak confinement), the entropy  $L$  saturates at a value that does not depend on  $\epsilon$  and is greater the larger is  $N$ . The value of  $g$  at which saturation takes place hardly depends on the number of particles, shifting only slightly towards larger values with increasing  $N$ .

The practical realizations of the model discussed in our work can be achieved experimentally in linear ion traps where the confining forces in the longitudinal direction are much softer than the radial confinement. In the case of singly charged ions the parameter  $g = ke^2 \sqrt{\frac{m}{\omega_x \hbar^3}}$ , where  $k$  is the Coulomb constant and  $m$  is the ion's mass, can be controlled by the axial trapping frequency  $\omega_x$ . In current experiments the values of  $\omega_x$  are below  $1 MHz$ , which corresponds to the crystalline phase with micrometer distances between the ions [21] and a value of  $g$  larger than  $10^6$ . In this regime, the correlation depends very weakly on anisotropy and the strictly one-dimensional approximation works well even at moderate values of  $\epsilon$ .

We think a more extensive analysis of the effects of anisotropy for a larger number of particles is desirable to get a deeper insight into the properties of strongly correlated bosons with Coulomb interaction.

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